



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:58 PM BST

PDB ID : 6P2A
Title : Chimera of bacteriophage OBP gp146 central spike protein and a T4 gp5 beta-helix fragment
Authors : Buth, S.A.; Shneider, M.M.; Leiman, P.G.
Deposited on : 2019-05-21
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

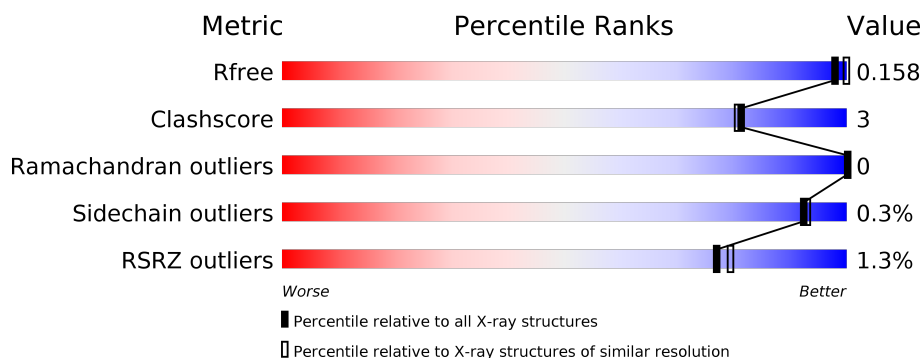
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	148	<div> <div>94%</div> <div> <div></div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	B	148	<div> <div>%</div> <div>93%</div> <div>5%</div> <div></div> </div>
1	C	148	<div> <div>%</div> <div>93%</div> <div>6%</div> <div></div> </div>
1	D	148	<div> <div>3%</div> <div>94%</div> <div></div> <div></div> </div>
1	E	148	<div> <div>%</div> <div>95%</div> <div></div> <div></div> </div>
1	F	148	<div> <div>%</div> <div>93%</div> <div>5%</div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PLM	F	702	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15142 atoms, of which 6858 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CHIMERA OF BACTERIOPHAGE OBP GP146 AND A T4 GP5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	145	Total	C	H	N	O	S	0	22	0
			2230	689	1088	206	243	4			
1	B	145	Total	C	H	N	O	S	0	21	0
			2257	698	1106	208	242	3			
1	C	146	Total	C	H	N	O	S	0	23	0
			2264	700	1107	207	246	4			
1	D	145	Total	C	H	N	O	S	0	28	0
			2337	722	1143	214	254	4			
1	E	145	Total	C	H	N	O	S	0	27	0
			2319	717	1134	213	251	4			
1	F	145	Total	C	H	N	O	S	0	17	0
			2214	687	1082	203	239	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	480	GLY	-	expression tag	UNP P16009
A	481	SER	-	expression tag	UNP P16009
A	482	GLY	-	expression tag	UNP P16009
A	483	SER	-	expression tag	UNP P16009
B	480	GLY	-	expression tag	UNP P16009
B	481	SER	-	expression tag	UNP P16009
B	482	GLY	-	expression tag	UNP P16009
B	483	SER	-	expression tag	UNP P16009
C	480	GLY	-	expression tag	UNP P16009
C	481	SER	-	expression tag	UNP P16009
C	482	GLY	-	expression tag	UNP P16009
C	483	SER	-	expression tag	UNP P16009
D	480	GLY	-	expression tag	UNP P16009
D	481	SER	-	expression tag	UNP P16009
D	482	GLY	-	expression tag	UNP P16009
D	483	SER	-	expression tag	UNP P16009

Continued on next page...

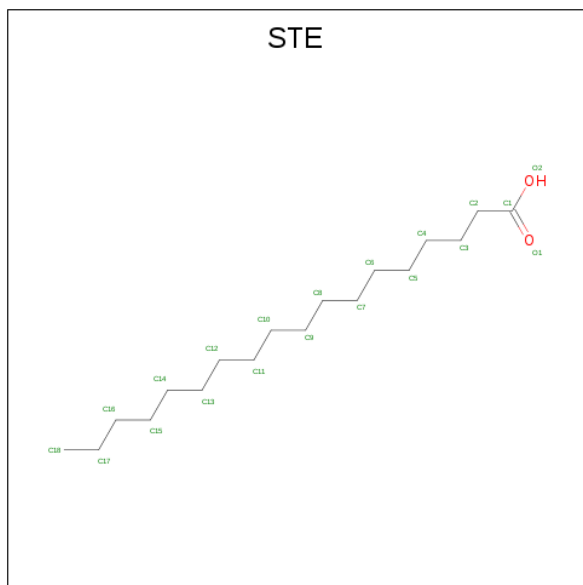
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	480	GLY	-	expression tag	UNP P16009
E	481	SER	-	expression tag	UNP P16009
E	482	GLY	-	expression tag	UNP P16009
E	483	SER	-	expression tag	UNP P16009
F	480	GLY	-	expression tag	UNP P16009
F	481	SER	-	expression tag	UNP P16009
F	482	GLY	-	expression tag	UNP P16009
F	483	SER	-	expression tag	UNP P16009

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

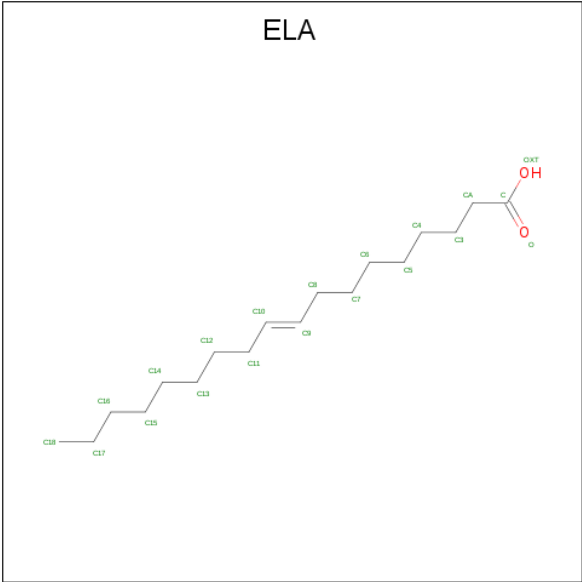
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is STEARIC ACID (three-letter code: STE) (formula: C₁₈H₃₆O₂).



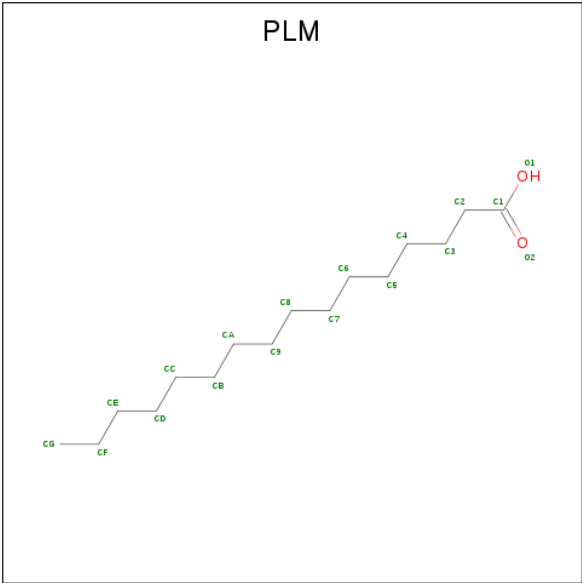
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 55 18 35 2	0	0
3	D	1	Total C H O 55 18 35 2	0	0

- Molecule 4 is 9-OCTADECENOIC ACID (three-letter code: ELA) (formula: C₁₈H₃₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			53	18	33	2		
4	F	1	Total	C	H	O	0	0
			53	18	33	2		

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			49	16	31	2		
5	F	1	Total	C	H	O	0	0
			49	16	31	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total 1	Mg 1	0	0
6	C	1	Total 1	Mg 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	189	Total 190	O 190	0	1
7	B	204	Total 205	O 205	0	1
7	C	225	Total 225	O 225	0	0
7	D	188	Total 189	O 189	0	1
7	E	195	Total 196	O 196	0	1
7	F	197	Total 198	O 198	0	1

3 Residue-property plots [i](#)

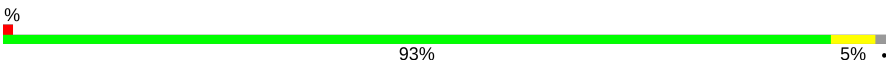
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: CHIMERA OF BACTERIOPHAGE OBP GP146 AND A T4 GP5

Chain A: 

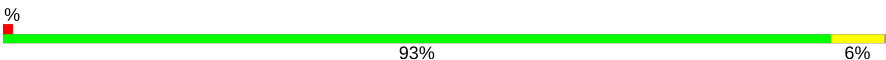


- Molecule 1: CHIMERA OF BACTERIOPHAGE OBP GP146 AND A T4 GP5

Chain B: 



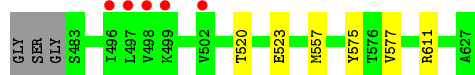
- Molecule 1: CHIMERA OF BACTERIOPHAGE OBP GP146 AND A T4 GP5

Chain C: 



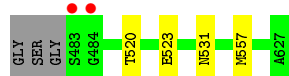
- Molecule 1: CHIMERA OF BACTERIOPHAGE OBP GP146 AND A T4 GP5

Chain D: 

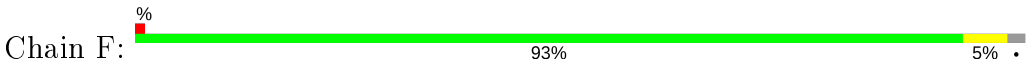


- Molecule 1: CHIMERA OF BACTERIOPHAGE OBP GP146 AND A T4 GP5

Chain E: 



- Molecule 1: CHIMERA OF BACTERIOPHAGE OBP GP146 AND A T4 GP5



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	140.01Å 140.01Å 63.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 1.90 49.50 – 1.86	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.50-1.90) 99.4 (49.50-1.86)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.127 , 0.158 0.127 , 0.158	Depositor DCC
R_{free} test set	5131 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15142	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: STE, MG, ELA, FE2, PLM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.72	0/1250	0.73	0/1691
1	B	0.67	0/1235	0.76	0/1667
1	C	0.68	0/1242	0.73	1/1676 (0.1%)
1	D	0.65	0/1279	0.73	0/1727
1	E	0.65	0/1274	0.75	0/1719
1	F	0.68	0/1206	0.73	0/1631
All	All	0.68	0/7486	0.74	1/10111 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	626	SER	N-CA-CB	-5.35	102.47	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1142	1088	993	6	0
1	B	1151	1106	1038	8	0
1	C	1157	1107	1024	8	0
1	D	1194	1143	1070	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1185	1134	1060	5	0
1	F	1132	1082	1027	9	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	20	35	35	3	0
3	D	20	35	35	0	0
4	A	20	33	33	3	0
4	F	20	33	33	0	0
5	B	18	31	31	2	0
5	F	18	31	31	2	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	190	0	0	3	4
7	B	205	0	0	1	5
7	C	225	0	0	4	2
7	D	189	0	0	2	3
7	E	196	0	0	3	2
7	F	198	0	0	3	1
All	All	8284	6858	6410	36	11

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:566:GLU:OE1	7:F:801:HOH:O	1.65	1.10
1:B:603:ASP:OD1	7:B:801:HOH:O	1.93	0.86
1:E:523[B]:GLU:OE1	1:F:531:ASN:ND2	2.08	0.86
1:A:557[B]:MET:SD	7:A:981:HOH:O	2.34	0.86
1:C:566:GLU:OE1	7:C:801:HOH:O	1.97	0.81
1:D:557[B]:MET:SD	7:D:971:HOH:O	2.44	0.74
1:C:568:ASN:OD1	7:C:802:HOH:O	2.06	0.73
1:F:568:ASN:OD1	7:F:802:HOH:O	2.07	0.73
1:E:557[B]:MET:SD	7:E:887:HOH:O	2.55	0.64
1:A:568:ASN:OD1	7:A:801:HOH:O	2.15	0.63
1:C:557[B]:MET:SD	7:C:1015:HOH:O	2.55	0.63
3:A:702:STE:H42	1:B:512:ILE:HG21	1.83	0.60
1:A:496:ILE:HD11	4:A:703:ELA:H121	1.83	0.58
1:D:523[B]:GLU:OE1	1:E:531:ASN:ND2	2.35	0.57
1:F:496:ILE:CG1	5:F:702:PLM:HE2	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:ILE:HD11	5:B:701:PLM:H31	1.90	0.54
1:A:512:ILE:HG21	4:A:703:ELA:H51	1.94	0.48
1:F:575:TYR:CZ	1:F:577[B]:VAL:CG2	2.98	0.47
1:B:512:ILE:CD1	5:B:701:PLM:H31	2.45	0.47
1:F:496:ILE:HG12	5:F:702:PLM:HE2	1.98	0.46
1:D:575:TYR:CE2	1:D:577[A]:VAL:CG2	2.99	0.45
4:A:703:ELA:H111	1:B:496[B]:ILE:HD13	1.97	0.45
1:A:570[B]:ASN:OD1	1:B:576:THR:OG1	2.36	0.44
1:D:520:THR:HG23	7:E:706:HOH:O	2.18	0.44
1:B:499:LYS:HD3	1:C:507[B]:GLU:OE1	2.18	0.43
1:D:611[B]:ARG:NH2	7:D:801:HOH:O	2.42	0.43
1:D:575:TYR:CZ	1:D:577[A]:VAL:CG2	3.02	0.43
1:F:575:TYR:CE2	1:F:577[B]:VAL:CG2	3.02	0.43
3:A:702:STE:H82	1:C:504:ILE:HD11	2.01	0.43
1:E:520:THR:HG23	7:F:903:HOH:O	2.18	0.42
7:E:743:HOH:O	1:F:576:THR:HG23	2.19	0.42
3:A:702:STE:H122	1:C:496:ILE:CD1	2.50	0.42
1:B:511:ASP:OD1	1:C:519:THR:OG1	2.30	0.42
1:C:611[A]:ARG:NH2	7:C:808:HOH:O	2.44	0.41
1:E:523[B]:GLU:O	1:F:531:ASN:HB2	2.20	0.41
1:A:570[B]:ASN:ND2	7:A:809:HOH:O	2.54	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:801:HOH:O	7:C:835:HOH:O[4_455]	1.63	0.57
7:B:949:HOH:O	7:B:985:HOH:O[3_564]	1.93	0.27
7:A:917:HOH:O	7:B:853:HOH:O[4_455]	2.00	0.20
7:D:940:HOH:O	7:F:982:HOH:O[3_554]	2.08	0.12
7:A:907:HOH:O	7:B:1001:HOH:O[4_455]	2.10	0.10
7:C:914:HOH:O	7:C:993:HOH:O[3_565]	2.12	0.08
7:D:895:HOH:O	7:D:948:HOH:O[2_554]	2.13	0.07
7:E:841:HOH:O	7:E:883:HOH:O[4_555]	2.15	0.05
7:A:838:HOH:O	7:A:938:HOH:O[3_564]	2.15	0.05
7:D:898:HOH:O	7:E:861:HOH:O[3_554]	2.16	0.04
7:A:906:HOH:O	7:B:899:HOH:O[3_564]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	165/148 (112%)	162 (98%)	3 (2%)	0	100	100
1	B	164/148 (111%)	161 (98%)	3 (2%)	0	100	100
1	C	167/148 (113%)	166 (99%)	1 (1%)	0	100	100
1	D	171/148 (116%)	170 (99%)	1 (1%)	0	100	100
1	E	170/148 (115%)	169 (99%)	1 (1%)	0	100	100
1	F	160/148 (108%)	159 (99%)	1 (1%)	0	100	100
All	All	997/888 (112%)	987 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/112 (116%)	128 (98%)	2 (2%)	65	62
1	B	127/112 (113%)	125 (98%)	2 (2%)	62	60
1	C	129/112 (115%)	129 (100%)	0	100	100
1	D	132/112 (118%)	132 (100%)	0	100	100
1	E	131/112 (117%)	131 (100%)	0	100	100
1	F	125/112 (112%)	125 (100%)	0	100	100
All	All	774/672 (115%)	770 (100%)	4 (0%)	92	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	554[A]	MET
1	A	554[B]	MET
1	B	554[A]	MET
1	B	554[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PLM	B	701	-	14,17,17	0.35	0	13,17,17	0.95	0
5	PLM	F	702	-	14,17,17	0.41	0	13,17,17	0.76	0
3	STE	A	702	-	16,19,19	0.29	0	15,19,19	0.97	0
4	ELA	F	701	-	16,19,19	0.30	0	15,19,19	0.38	0
4	ELA	A	703	-	16,19,19	0.26	0	15,19,19	0.60	0
3	STE	D	703	-	16,19,19	0.38	0	15,19,19	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PLM	B	701	-	-	5/13/15/15	-
5	PLM	F	702	-	-	6/13/15/15	-
3	STE	A	702	-	-	10/15/17/17	-
4	ELA	F	701	-	-	8/15/17/17	-
4	ELA	A	703	-	-	9/15/17/17	-
3	STE	D	703	-	-	10/15/17/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	703	STE	C1-C2-C3-C4
4	F	701	ELA	C14-C15-C16-C17
3	A	702	STE	C11-C10-C9-C8
4	A	703	ELA	C14-C15-C16-C17
4	A	703	ELA	C10-C11-C12-C13
3	A	702	STE	C3-C4-C5-C6
3	A	702	STE	C2-C3-C4-C5
4	F	701	ELA	CA-C3-C4-C5
3	D	703	STE	C3-C4-C5-C6
3	D	703	STE	C14-C15-C16-C17
5	B	701	PLM	CA-CB-CC-CD
4	A	703	ELA	C13-C14-C15-C16
4	F	701	ELA	C4-C5-C6-C7
3	A	702	STE	C5-C6-C7-C8
3	A	702	STE	C14-C15-C16-C17
3	D	703	STE	C13-C14-C15-C16
4	A	703	ELA	C11-C12-C13-C14
4	A	703	ELA	C12-C13-C14-C15
5	F	702	PLM	C6-C7-C8-C9
4	A	703	ELA	C3-C4-C5-C6
4	F	701	ELA	C5-C6-C7-C8
4	A	703	ELA	C4-C5-C6-C7
5	F	702	PLM	CB-CC-CD-CE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	701	PLM	CB-CC-CD-CE
3	D	703	STE	C4-C5-C6-C7
3	A	702	STE	C13-C14-C15-C16
4	F	701	ELA	C3-C4-C5-C6
3	A	702	STE	C12-C13-C14-C15
4	F	701	ELA	C12-C13-C14-C15
3	D	703	STE	C9-C10-C11-C12
4	A	703	ELA	C5-C6-C7-C8
5	F	702	PLM	CD-CE-CF-CG
5	F	702	PLM	CA-CB-CC-CD
4	F	701	ELA	C13-C14-C15-C16
3	A	702	STE	C9-C10-C11-C12
3	D	703	STE	C11-C10-C9-C8
5	F	702	PLM	C7-C8-C9-CA
3	D	703	STE	C6-C7-C8-C9
3	A	702	STE	C10-C11-C12-C13
4	F	701	ELA	C11-C12-C13-C14
5	F	702	PLM	CC-CD-CE-CF
3	A	702	STE	C7-C8-C9-C10
5	B	701	PLM	C7-C8-C9-CA
3	D	703	STE	C12-C13-C14-C15
5	B	701	PLM	C6-C7-C8-C9
4	A	703	ELA	CA-C3-C4-C5
5	B	701	PLM	C3-C4-C5-C6
3	D	703	STE	C11-C12-C13-C14

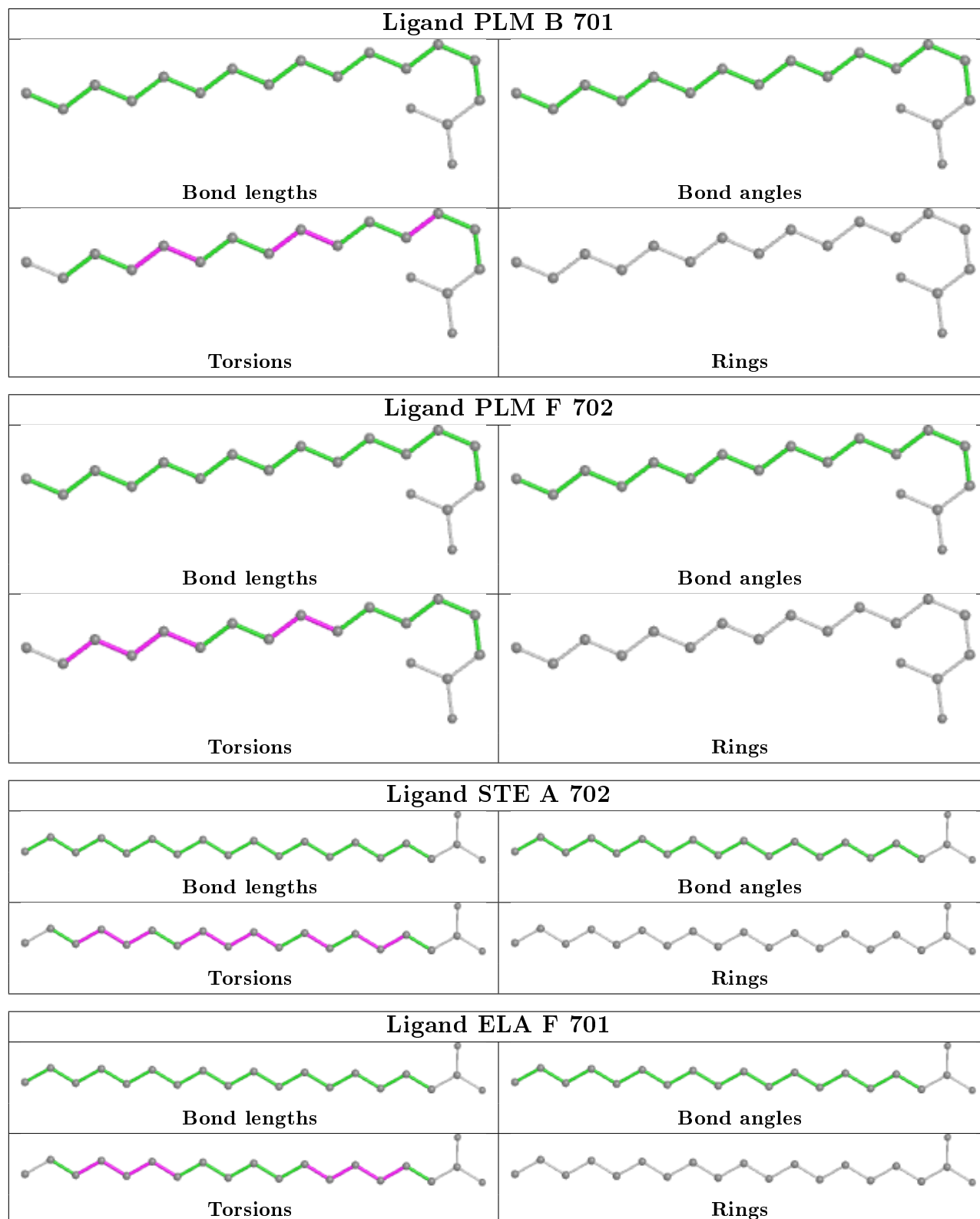
There are no ring outliers.

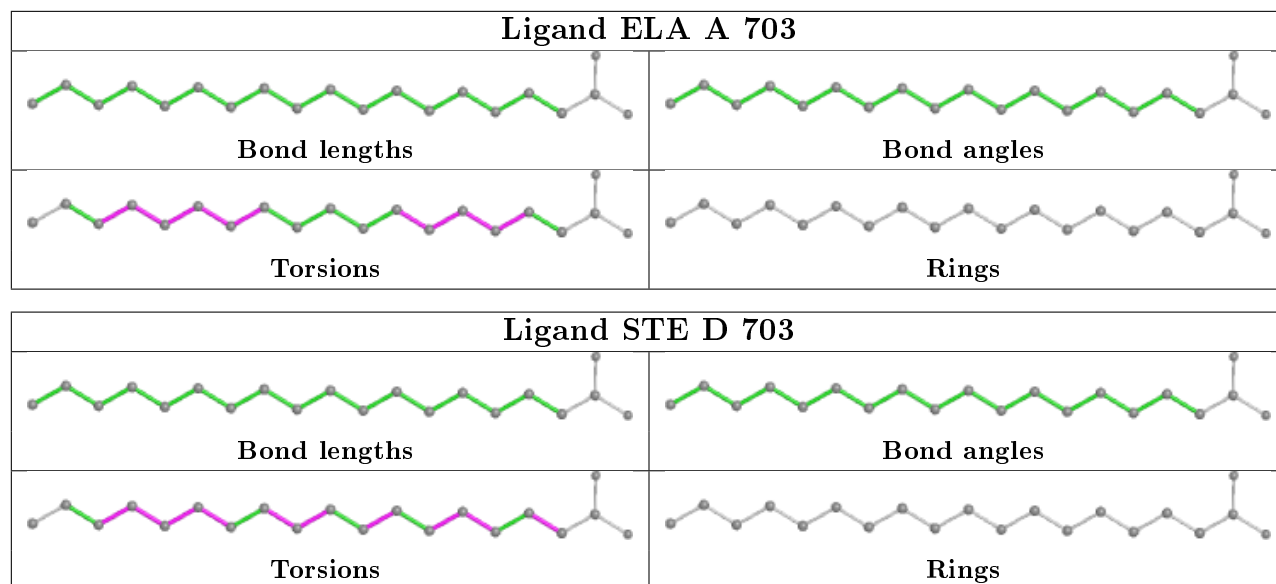
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	701	PLM	2	0
5	F	702	PLM	2	0
3	A	702	STE	3	0
4	A	703	ELA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	145/148 (97%)	-0.47	0 100 100	10, 23, 45, 97	0
1	B	145/148 (97%)	-0.46	1 (0%) 87 88	10, 23, 50, 101	0
1	C	146/148 (98%)	-0.43	1 (0%) 87 88	11, 23, 47, 82	0
1	D	145/148 (97%)	-0.35	5 (3%) 45 48	11, 22, 47, 99	0
1	E	145/148 (97%)	-0.34	2 (1%) 75 77	11, 23, 51, 92	0
1	F	145/148 (97%)	-0.29	2 (1%) 75 77	11, 23, 52, 89	0
All	All	871/888 (98%)	-0.39	11 (1%) 77 79	10, 23, 50, 101	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	483	SER	3.3
1	D	496[A]	ILE	3.3
1	F	490	VAL	3.2
1	B	483	SER	2.8
1	D	498	VAL	2.4
1	D	499	LYS	2.4
1	D	497[A]	LEU	2.2
1	C	482	GLY	2.2
1	D	502	VAL	2.1
1	F	492	GLY	2.1
1	E	484	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

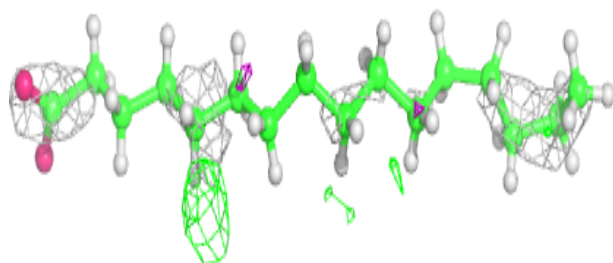
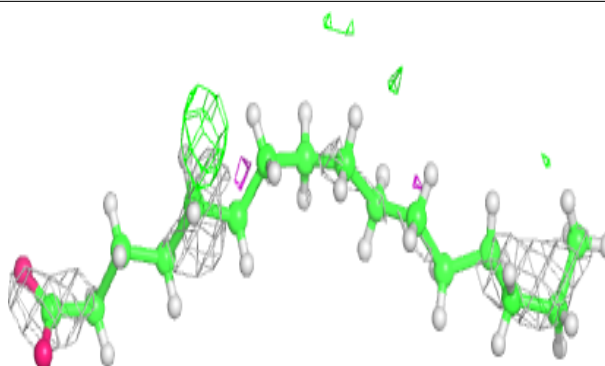
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PLM	F	702	18/18	0.70	0.52	59,84,99,99	0
5	PLM	B	701	18/18	0.79	0.38	56,81,96,102	0
3	STE	A	702	20/20	0.82	0.39	39,77,93,93	0
4	ELA	F	701	20/20	0.82	0.29	54,75,94,97	0
3	STE	D	703	20/20	0.83	0.33	55,77,96,105	0
4	ELA	A	703	20/20	0.87	0.29	56,75,101,101	0
2	FE2	D	701	1/1	0.99	0.10	13,13,13,13	0
6	MG	C	701	1/1	1.00	0.03	22,22,22,22	0
2	FE2	A	701	1/1	1.00	0.12	12,12,12,12	0
6	MG	D	702	1/1	1.00	0.10	21,21,21,21	0

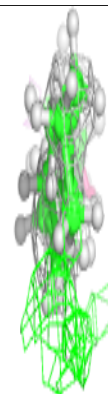
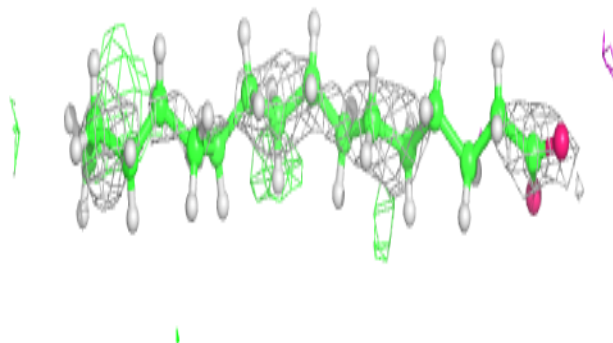
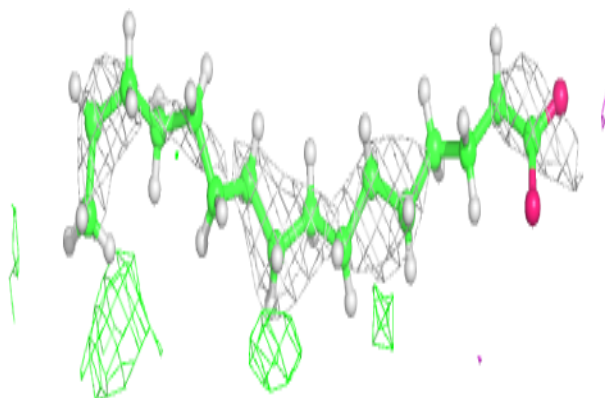
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PLM F 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

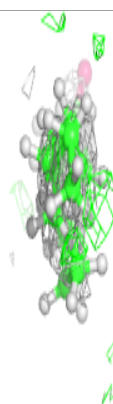
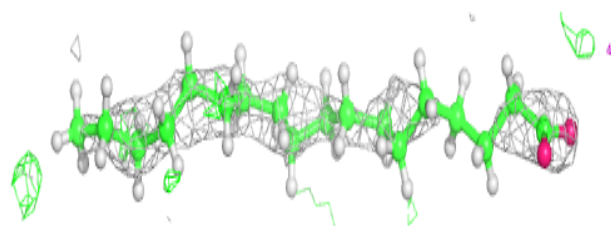
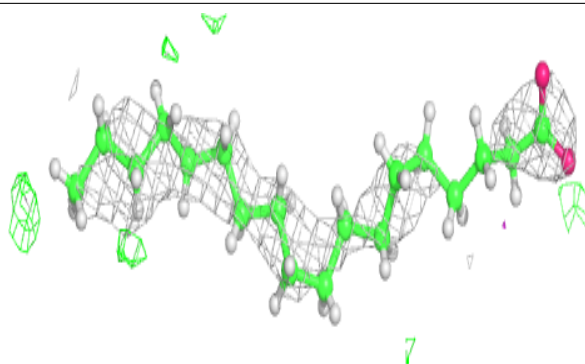
**Electron density around PLM B 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

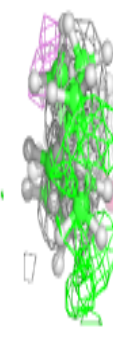
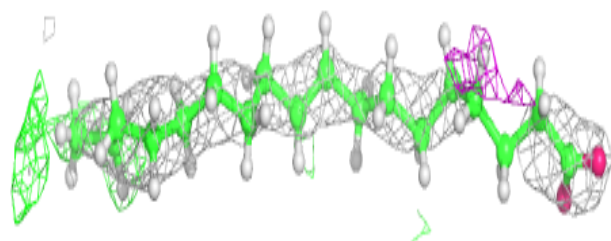
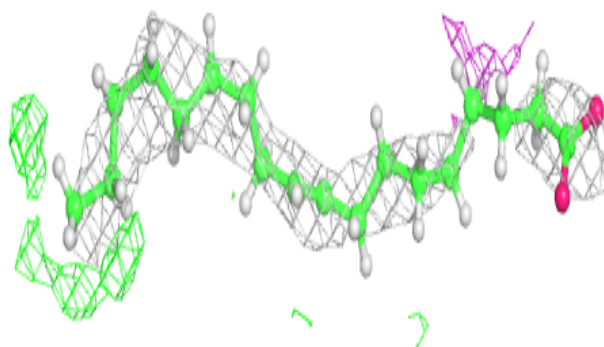


Electron density around STE A 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

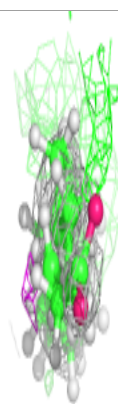
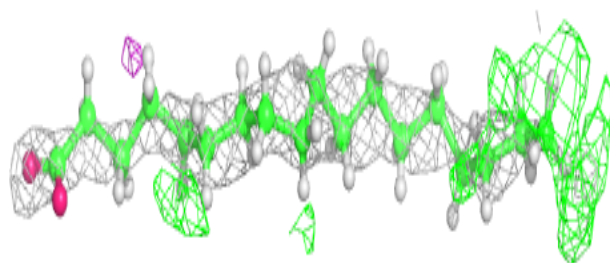
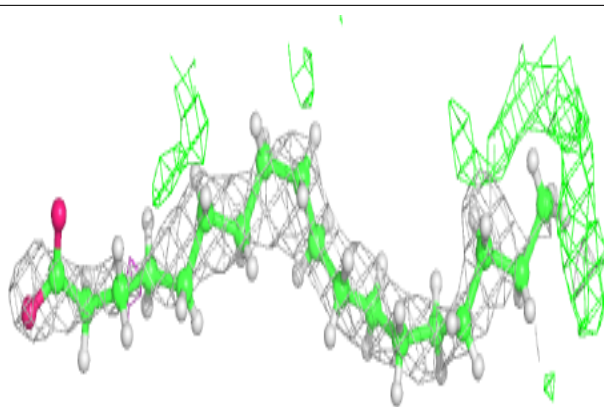
**Electron density around ELA F 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

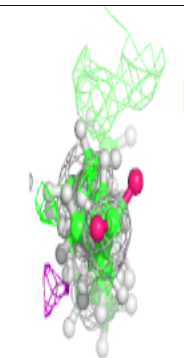
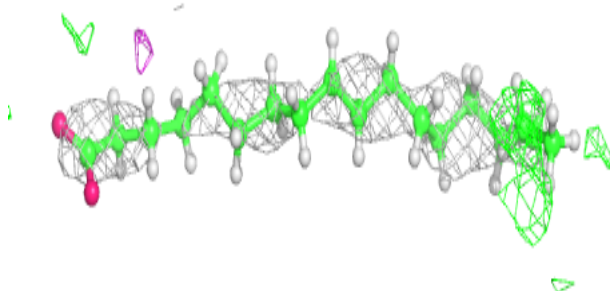
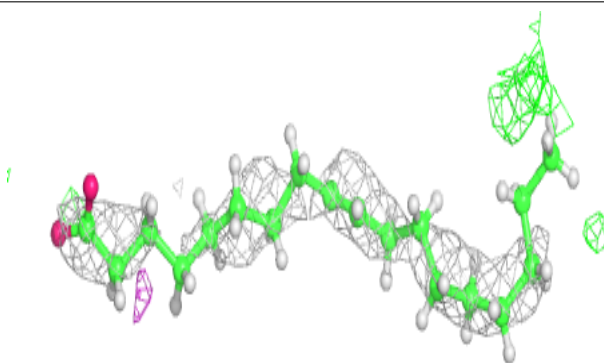


Electron density around STE D 703:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ELA A 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.